Machine Learning on Large-Scale Graphs

Graph Limits, Nonparametric Models, and Estimation Workshop

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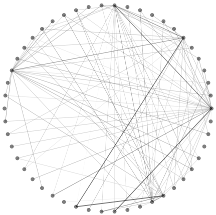
Simons / FODSI / JHU

Thanks to Luiz Chamon (U. Stuttgart) and Alejandro Ribeiro (UPenn)

Machine Learning on Large-Scale Graphs

- The why: need to process information on very large graphs in a wide range of applications

  $\Rightarrow$ E.g., product recommendation systems, control of teams of autonomous agents



product similarity graph

robot swarm (Tolstaya, E. et al., 2019)

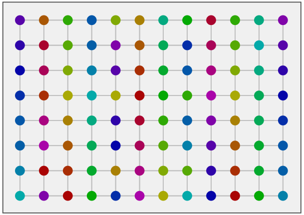
- Machine learning is solution of choice $\Rightarrow$ has been shown to outperform other existing solutions

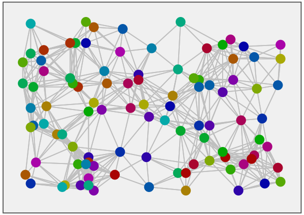
Graph Neural Networks

- The how: empirical and theoretical evidence to support using neural networks

  $\Rightarrow$ Standard neural networks are not scalable $\Rightarrow$ use convolutional neural networks (CNNs)

- But convolutional neural networks only operate on regular, grid-like data...





- ... and we would like to process information on irregular structures better modeled as graphs

  $\Rightarrow$ Graph convolutions and graph neural networks (GNNs) (Kipf, T., Welling, M., 2017)

Do Graph Neural Networks Scale?

Q1: We have empirically observed that GNNs scale. Why do they scale?

Q2: Can success of GNNs on moderate-size graphs be used to create success at large-scale?

- To answer these questions, turn to CNNs $\Rightarrow$ known to scale well for images and time sequences

Convolutional Neural Networks Have Limits

- Discrete time/image signals converge to continuous time/image signals $\Rightarrow \downarrow$ intrinsic dimension

143 × 95 → 205 × 136 → 294 × 195 → 600 × 399

$\Rightarrow$ From SP theory, CNNs have well-defined limits on the limits of images and time signals

- A1: Intrinsic dimensionality of the problem is less than the size of the image
- A2: Training with small images is sufficient $\Rightarrow$ CIFAR 10 images are 32×32

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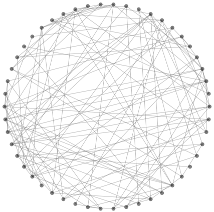
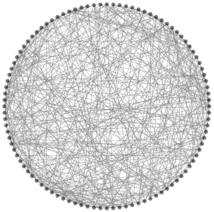
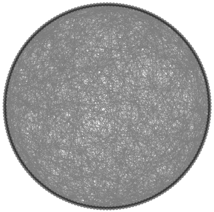
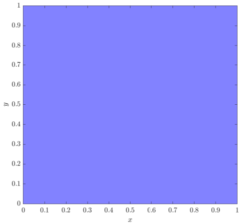
Graphons

- Graphs also have limit objects that effectively limit their dimensionality $\Rightarrow$ one is the graphon

$n = 50$ nodes $\rightarrow$ $n = 100$ nodes $\rightarrow$ $n = 200$ nodes $\rightarrow$ Graphon $W(u, v) = p$

- A graphon can be thought of as a graph with an uncountable number of nodes

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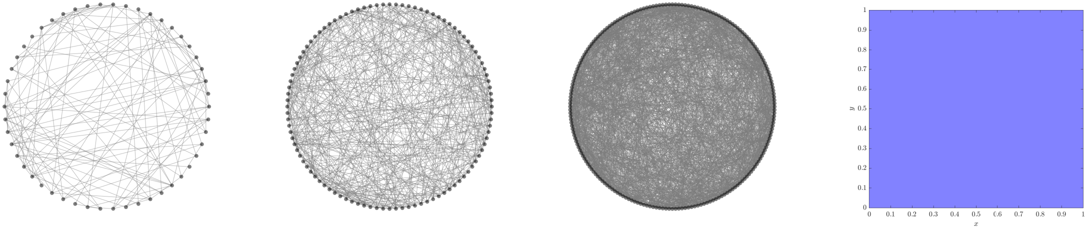

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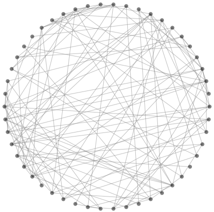

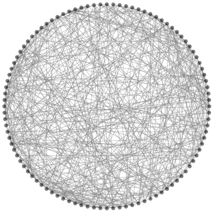

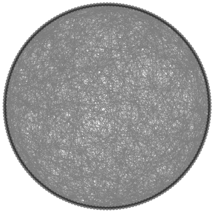

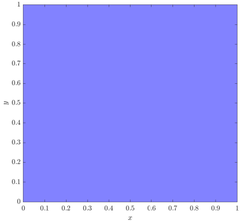

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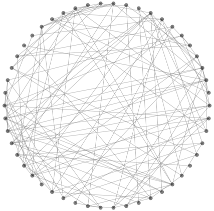

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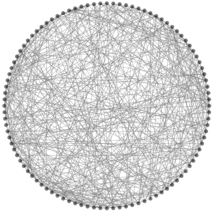

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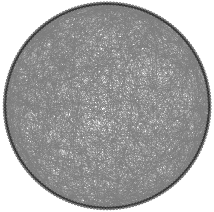

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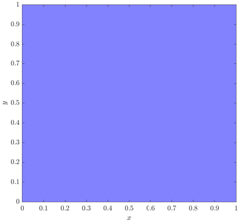

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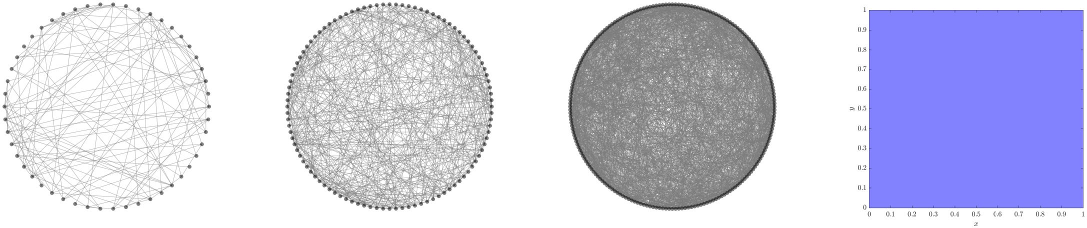

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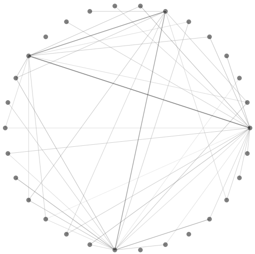
- A graphon can be thought of as a graph with an uncountable number of nodes

- Graphs however do not have the Euclidean structure time and image signals have in the limit



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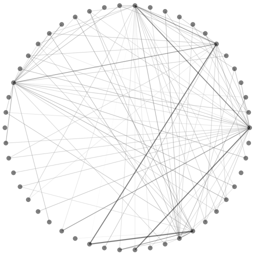

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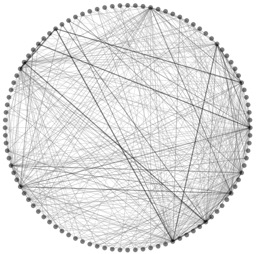

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- So do graph convolutions and graph neural networks converge to limits on the graphon?

Large-Scale Graphs

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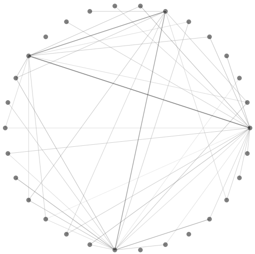

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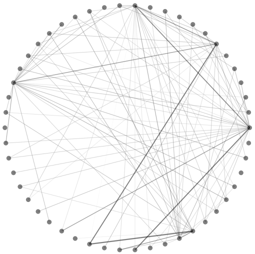

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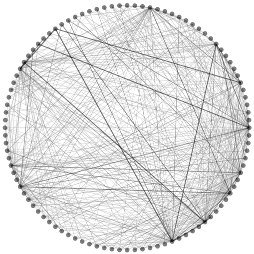

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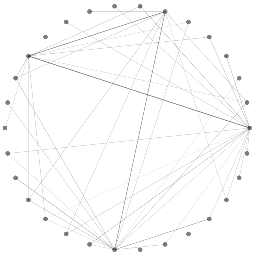

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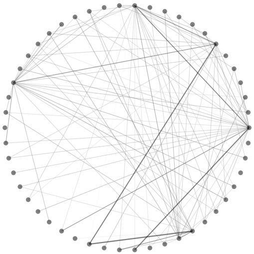

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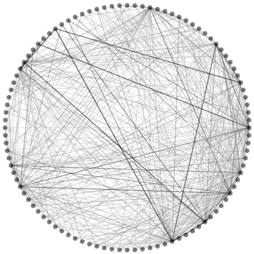

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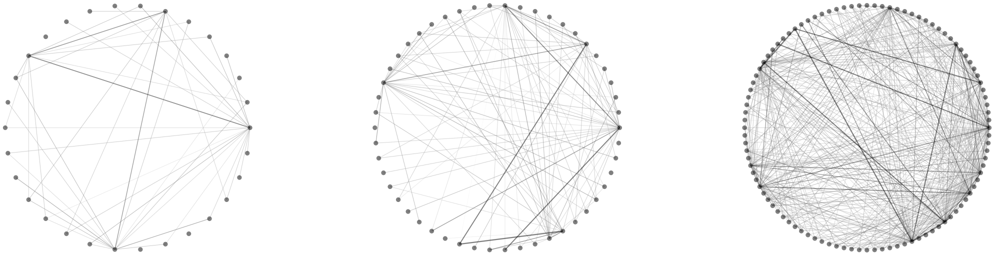

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- So do graph convolutions and graph neural networks converge to limits on the graphon?

Graph Neural Networks Have Limits

Q1: We have empirically observed that GNNs scale. Why do they scale?

- A1: Because graph convolutions and GNNs have well-defined limits on graphons

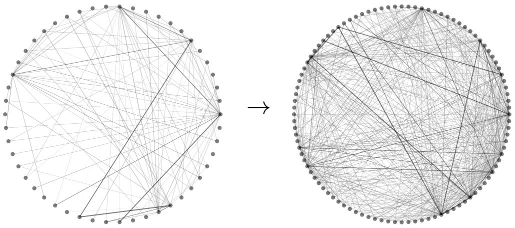
Ruiz, L., Chamon, L. F. O., Ribeiro, A., *Graphon Signal Processing,* IEEE TSP, 2021

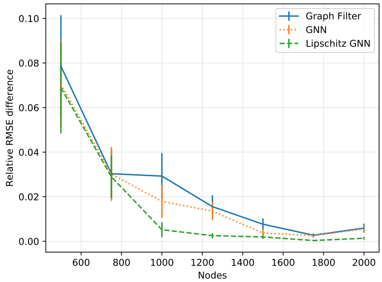
Q2: Can success of GNNs on moderate-size graphs be used to create success at large-scale?

- A2: Yes, as GNNs are transferable $\Rightarrow$ can be trained on moderate-size and executed on large-scale

Ruiz, L., Chamon, L. F. O., Ribeiro, A., *Transferability Properties of Graph Neural Networks,* Submitted to IEEE TSP

- Transferability of graph neural networks useful in practice $\Rightarrow$ recommendation system

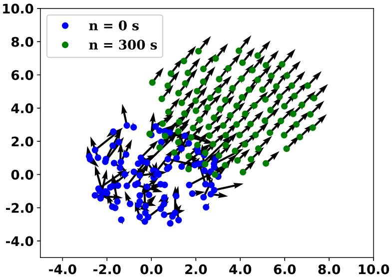


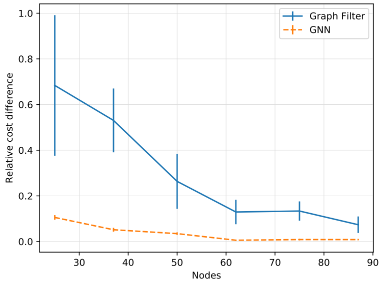


- Performance difference on training and target graphs decreases as size of training graph grows
- GNNs appear to be more transferable than graph convolutional filters $\Rightarrow$ better ML model

Transferability of Graph Neural Networks

- Transferability of graph neural networks useful in practice $\Rightarrow$ decentralized robot control





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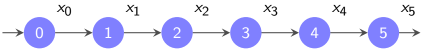
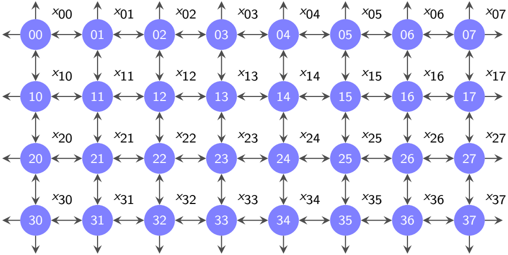
Graph Convolutions

- Use line and grid graphs to write convolutions as polynomials on respective adjacency matrices $\mathbf{S}$

Description of time with a directed line graph



Description of images (space) with a grid graph



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Convolutions in Time and Space

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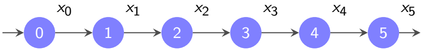

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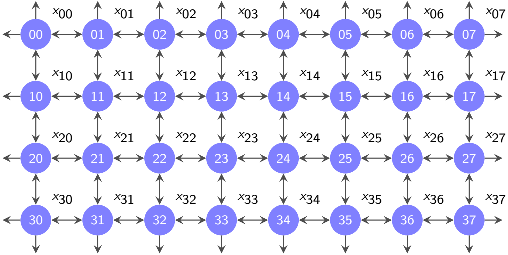

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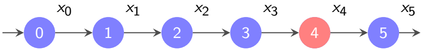

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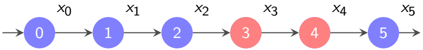

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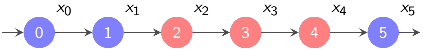

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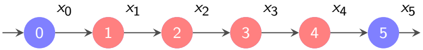

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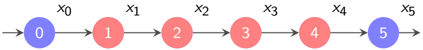

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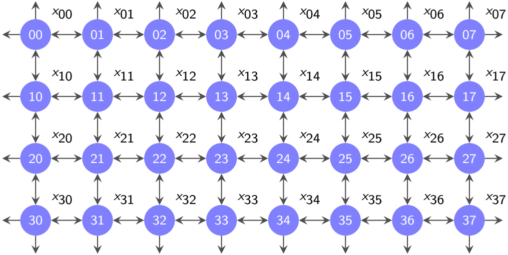

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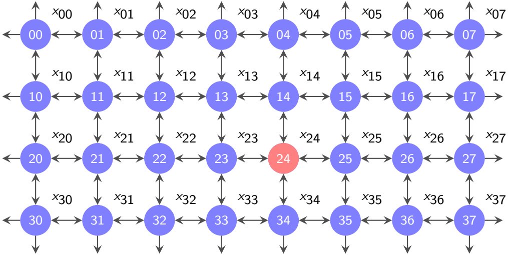

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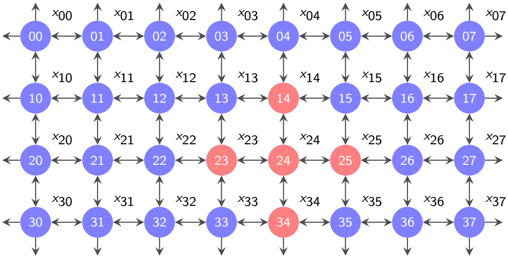

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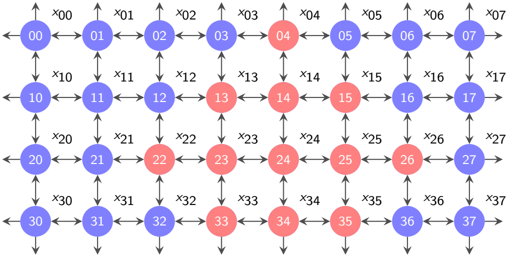
Description of images (space) with a grid graph



- Filter with coefficients h_k $\Rightarrow$ Output $\mathbf{z} = \; h_0\,\mathbf{S}^0\mathbf{x} \; + h_1\,\mathbf{S}^1\mathbf{x} \; + h_2\,\mathbf{S}^2\mathbf{x} \; + h_3\,\mathbf{S}^3\mathbf{x} \; + \ldots = \sum_{k=0}^{K-1} h_k\,\mathbf{S}^k\mathbf{x}$

- Use line and grid graphs to write convolutions as polynomials on respective adjacency matrices $\mathbf{S}$

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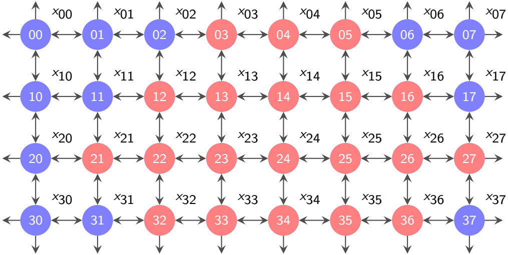

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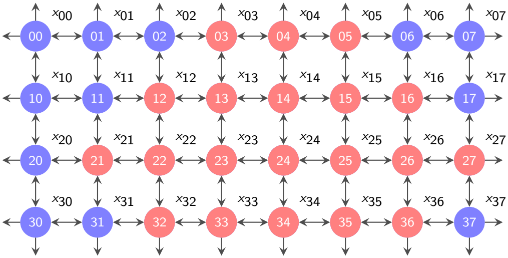

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Convolutions in Time and Space

- Use line and grid graphs to write convolutions as polynomials on respective adjacency matrices $\mathbf{S}$

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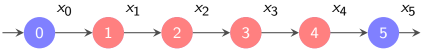

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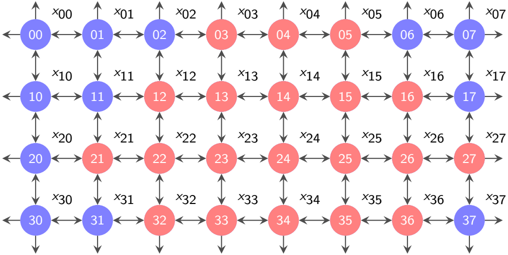

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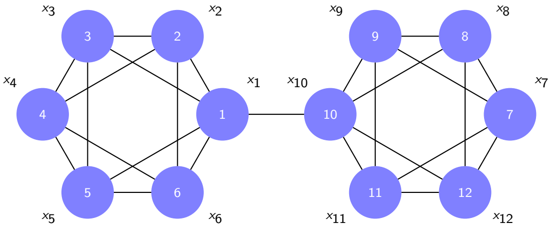
Convolutions on Graphs

- For graph signals we define graph convolutions as polynomials on matrix representations of graphs



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- To analyze their convergence to a limit object on the graphon $\Rightarrow$ need to define graphons

Ortega, A., Frossard, P., Kovačević, J., Moura, J. M. F, Vandergheynst, P., *Graph Signal Processing*, Proc. IEEE, 2018

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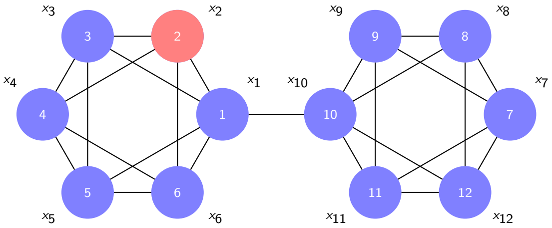

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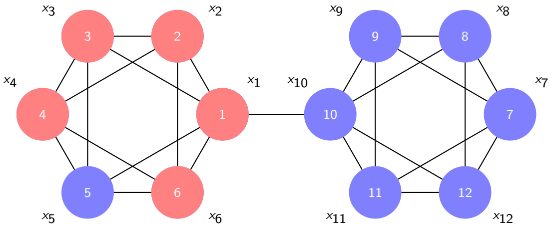

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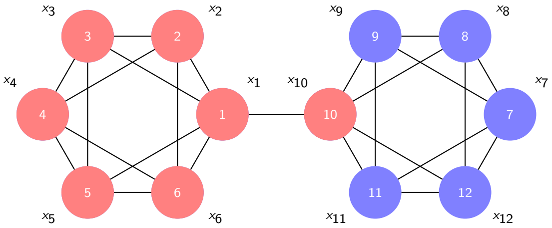

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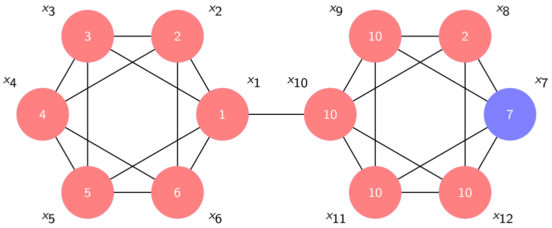

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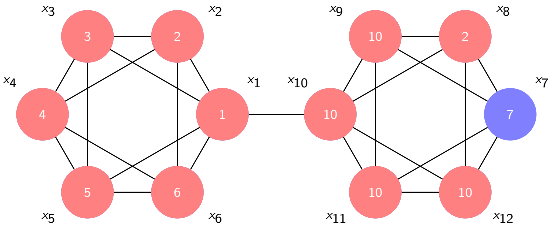

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Graphons

Definition (Graphon) (Borgs, C., Chayes, J., Lovász, L., Sós, V., Vesztergombi, K., 2008)

A graphon **W** is a bounded symmetric measurable function $\Rightarrow \mathbf{W} : [0,1]^2 \to [0,1]$

- Can think of a graphon as a weighted symmetric graph with an uncountable number of nodes

  $\Rightarrow$ Labels are graphon arguments $u \in [0,1]$, weights are graphon values $W(u,v) = W(v,u)$

- Interpreted as the limit of a sequence of graphs in the sense that densities of motifs converge

- Interpreted as a generative model of graph families by sampling edges $(u_i, u_j) \sim \mathcal{B}(\mathbf{W}(u_i, u_j))$

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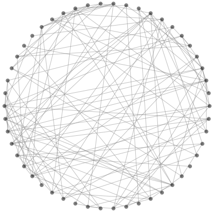
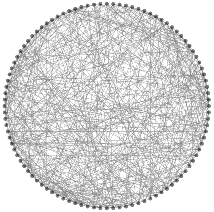
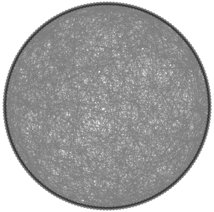
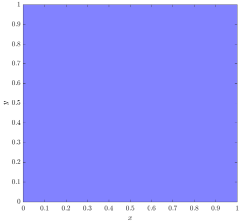
Uniform Graphon as a Limit Object

- A sequence of Erdős-Rényi graphs converges to Erdős-Rényi graphons









$n = 50$ nodes $\rightarrow$ $n = 100$ nodes $\rightarrow$ $n = 200$ nodes $\rightarrow$ Graphon $W(u, v) = p$

- The Erdős-Rényi graphon can be used to sample uniform graphs with 200, 100, and 50 nodes

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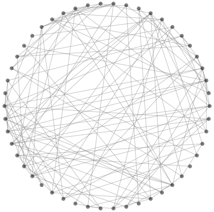

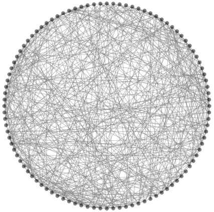

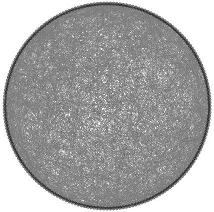

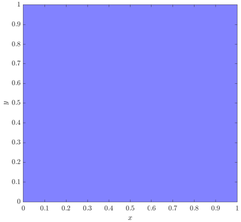

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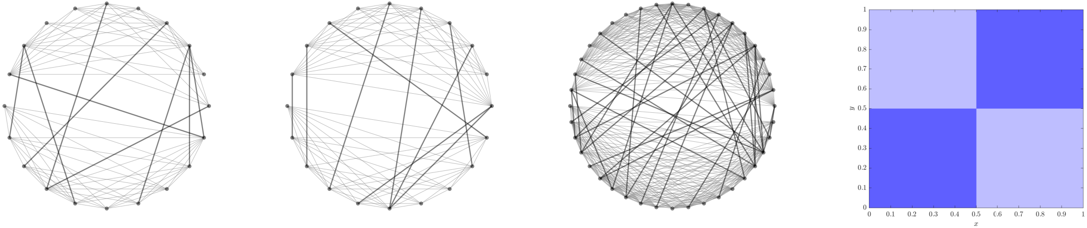
SBM as a Limit Object

- A sequence of stochastic block model graphs converges to stochastic block model graphons



$n = 20$ nodes $\rightarrow$ $n = 30$ nodes $\rightarrow$ $n = 40$ nodes $\rightarrow$ Graphon $W(u, v)$

- The stochastic block model graphon can be used to sample SBM graphs with 40, 30, and 20 nodes

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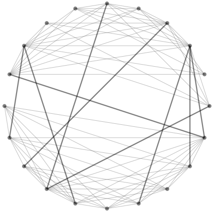
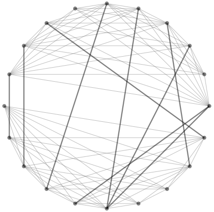
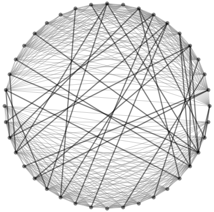
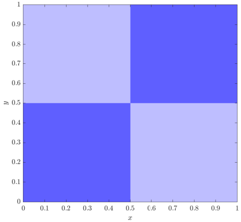

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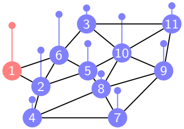
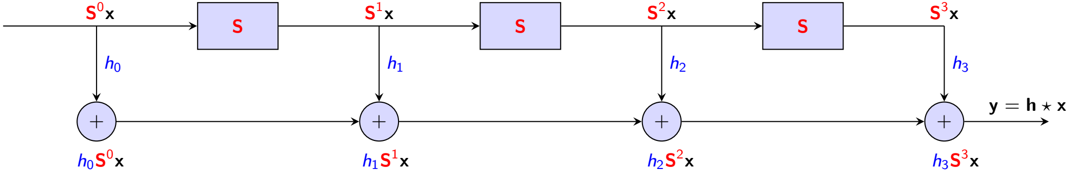
Graphon Convolutions

Convolutions on Graphs

- Graph convolution $\Rightarrow$ Output $\mathbf{z} = \; h_0\,\mathbf{S}^0\mathbf{x} \; + h_1\,\mathbf{S}^1\mathbf{x} \; + h_2\,\mathbf{S}^2\mathbf{x} \; + h_3\,\mathbf{S}^3\mathbf{x} \; + \ldots = \sum_{k=0}^{K-1} h_k\,\mathbf{S}^k\mathbf{x}$





- Note that the graph convolution is parametrized by the operator $\mathbf{z}_k = \mathbf{S}\mathbf{z}_{k-1}$ $\Rightarrow$ graph shift operator

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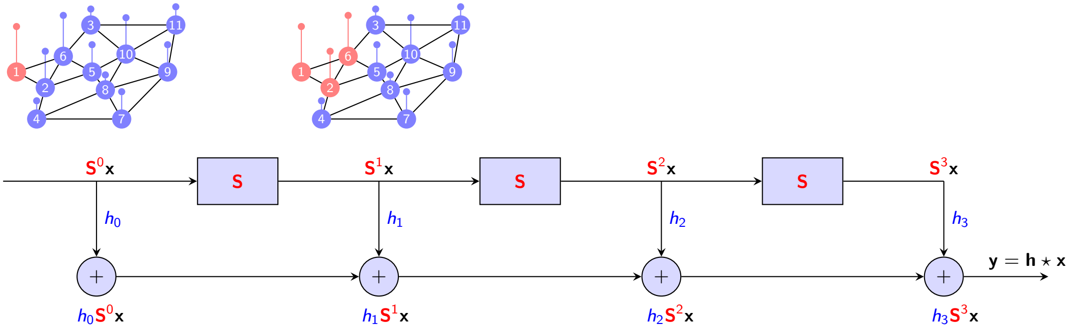

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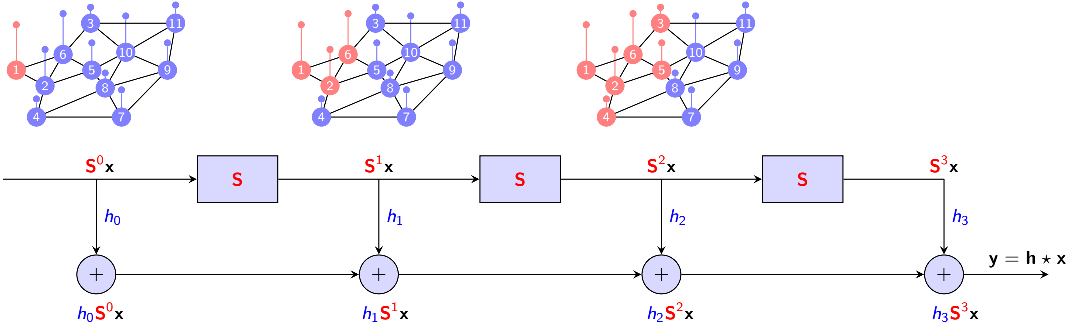

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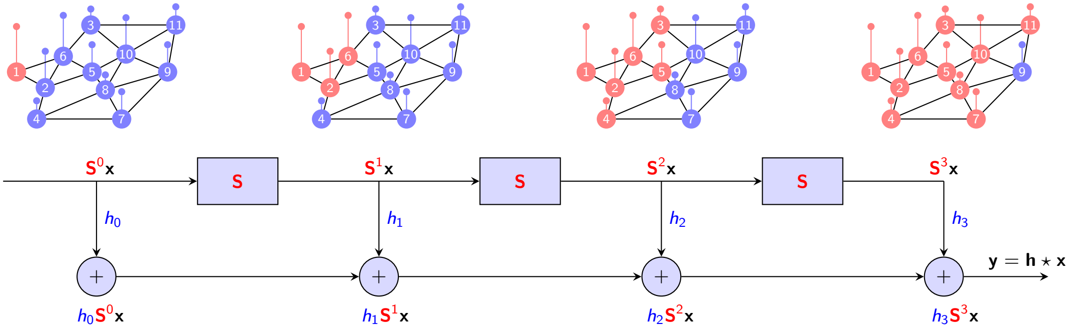

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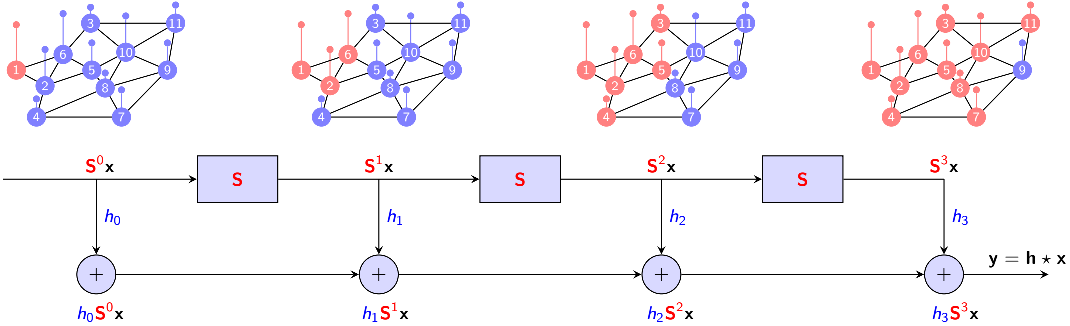

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- Graphon convolutions are analogously parametrized by the graphon shift operator

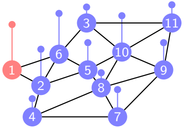
Definition (Graphon Shift Operator) (Ruiz, L., Chamon, L. F. O., Ribeiro A., TSP'21)

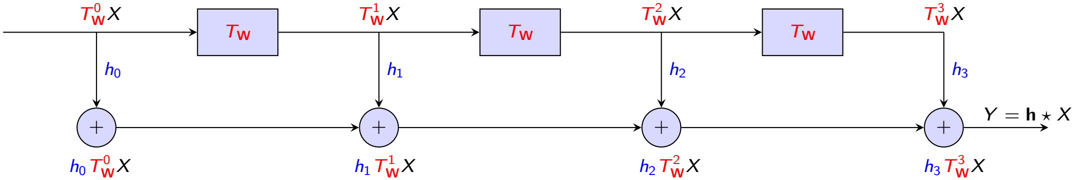
The graphon shift operator of a graphon $\mathbf{W}$ is defined as

$$Y(v) = (T_{\mathbf{W}}X)(v) = \int_0^1 \mathbf{W}(u, v)X(u)du.$$

- The graphon shift operator is an integral linear operator with kernel given by the graphon $\mathbf{W}$

- Graphon convolution $\Rightarrow Z = h_0 \, T_{\mathbf{W}}^0 X + h_1 \, T_{\mathbf{W}}^1 X + h_2 \, T_{\mathbf{W}}^2 X + h_3 \, T_{\mathbf{W}}^3 X \, \ldots = \sum_{k=0}^{K-1} h_k \, T_{\mathbf{W}}^k X$





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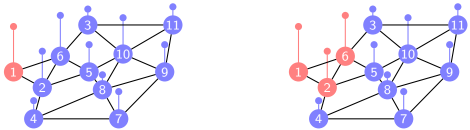

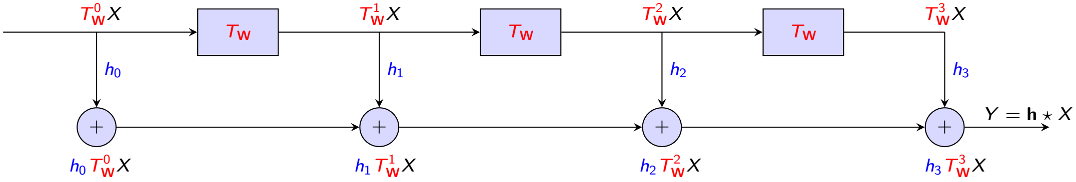

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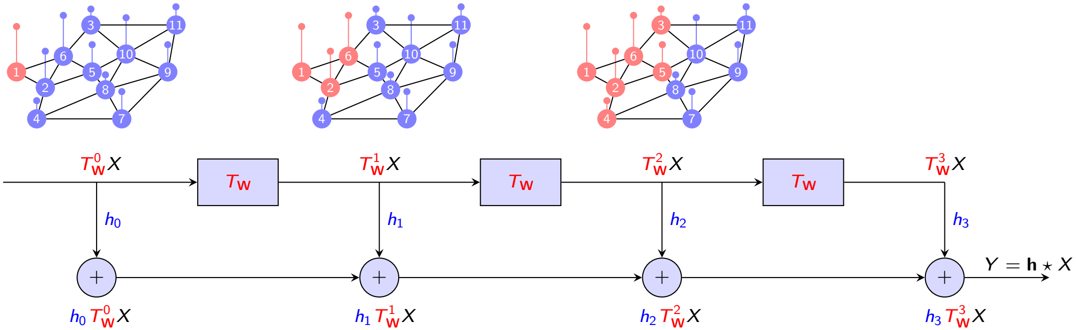

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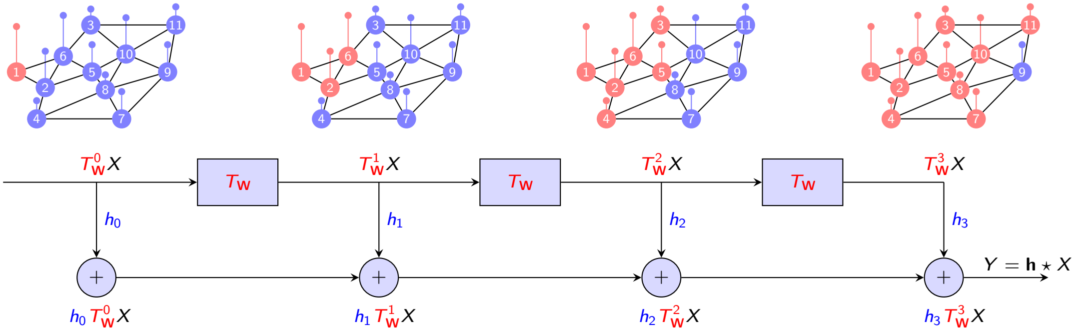

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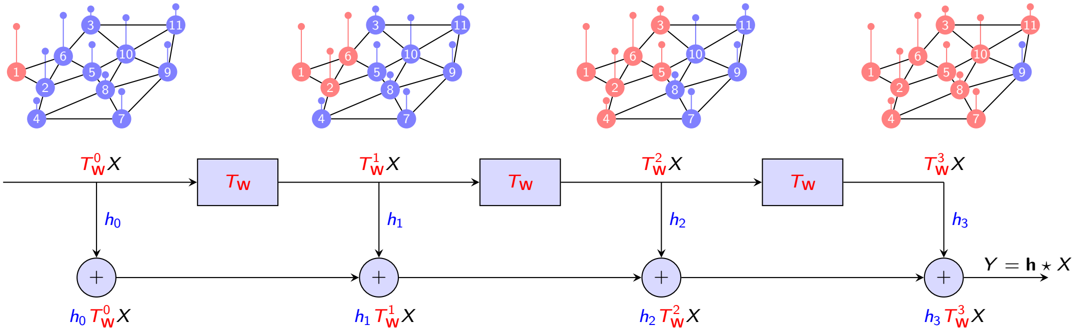


Frequency Representation of Graph Filters

- The graph (which is symmetric) admits the eigenvector decomposition $\mathbf{S}_n = \mathbf{V}_n \mathbf{\Lambda}_n \mathbf{V}_n^H$

Theorem (Graph frequency representation of graph filters)

Consider graph filter with coefficients h_k, graph signal $\mathbf{x}_n$ and the filtered signal $\mathbf{y}_n = \sum_{k=0}^{K-1} h_k \mathbf{S}_n^k \mathbf{x}_n$.

The Graph Fourier Transforms $\tilde{\mathbf{x}}_n = \mathbf{V}_n^H \mathbf{x}_n$ and $\tilde{\mathbf{y}}_n = \mathbf{V}_n^H \mathbf{y}_n$ are related by

$$\tilde{y}_{nj} = \sum_{k=0}^{K-1} h_k \lambda_{nj}^k \tilde{x}_{nj} \qquad \Rightarrow \qquad \tilde{h}(\lambda) = \sum_{k=0}^{K-1} h_k \lambda^k$$

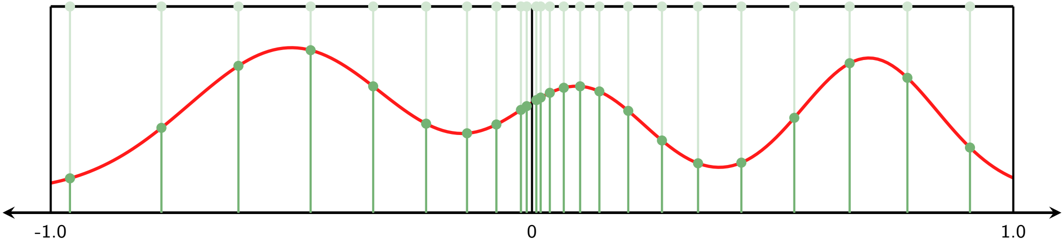
- This is a simple eigenvalue decomposition of the graph filter polynomial $\Rightarrow$ Nonetheless interesting

  $\Rightarrow$ It is not only that the operator is pointwise, it also decouples the filter from the graph

Graph Frequency Response

- The frequency response is independent of the graph. It is a polynomial on a scalar variable λ

- Graph determines eigenvalues at which response is instantiated $\Rightarrow \tilde{y}_{nj} = \sum_{k=0}^{K-1} h_k \lambda_{nj}^k \tilde{x}_{nj} = h(\lambda_{nj})\tilde{x}_{nj}$



- Since graphon shifts are Hilbert-Schmidt operators, the same can be done for graphon filters
- The eigenfunction representation of the graphon shift is $W(u, v) = \sum_{j \in \mathbb{Z} \setminus \{0\}} \lambda_j \phi_j(u) \varphi_j(v)$

Theorem (Graphon frequency representation of graphon filters)

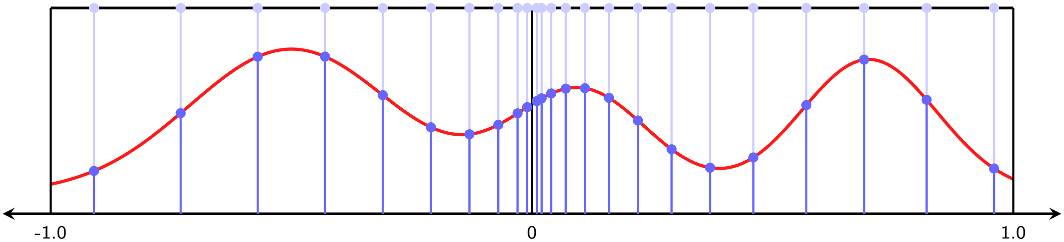
Consider graphon filter with coefficients h_k, graphon signal X and the filtered signal Y. The Graphon Fourier Transforms $\tilde{X}_j = \int_0^1 \varphi_j(u) X(u) du$ and $\tilde{Y}_j = \int_0^1 \varphi_j(u) Y(u) du$ are related by

$$\tilde{Y}_j = \sum_{k=0}^{K-1} h_k \lambda_j^k \tilde{X}_j \qquad \Rightarrow \qquad \tilde{h}(\lambda) = \sum_{k=0}^{K-1} h_k \lambda^k$$

- Like graph filters, graphon filters have pointwise spectra and are decoupled from the graphon

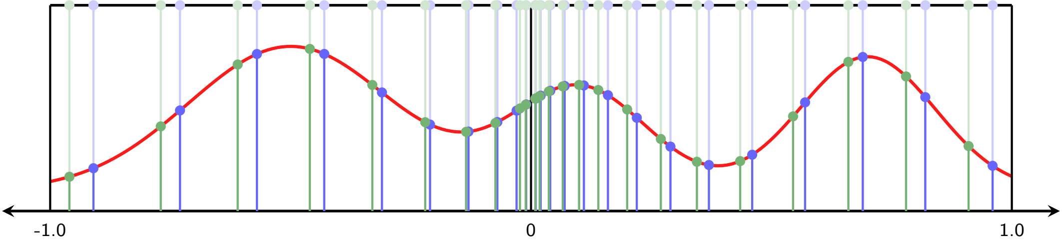
Graph Frequency Response

- Graphon-independent. More importantly the same as the graph response for the same coefficients h_k
- Graphon determines eigenvalues at which response is instantiated $\Rightarrow \tilde{Y}_j = \sum_{k=0}^{K-1} h_k \lambda_j^k \tilde{X}_j = h(\lambda_j)\tilde{X}_j$



Spectral Representation of the Graph and Graphon Convolution

- Spectral response of graph and graphon convolution is given by the same function $h(\lambda)$



- Spectral response of the graph convolution determined by evaluating $h(\lambda)$ at graph eigenvalues

- Spectral response of the graphon convolution determined by evaluating $h(\lambda)$ at graphon eigenvalues

Convergence of Graph Convolutions

- Graph convolutions converge to graphon convolutions $\Rightarrow$ provided that $h(\lambda)$ is Lipschitz

Theorem (Convergence of Graph Convolutions) (Ruiz, L. et al., EUSIPCO'20, TSP'21)

Given convergent graph signal sequence $(G_n, \mathbf{x}_n) \to (W, X)$ and convolutions $\mathbf{H}(\mathbf{S}_n)$ and T_H

generated by the same coefficients h_k, if the spectral response $h(\lambda)$ is Lipschitz,

$$(\mathbf{G}_n, \mathbf{y}_n) \to (\mathbf{W}, Y)$$

i.e., the sequence of output graph signals converges to the output graphon signal.

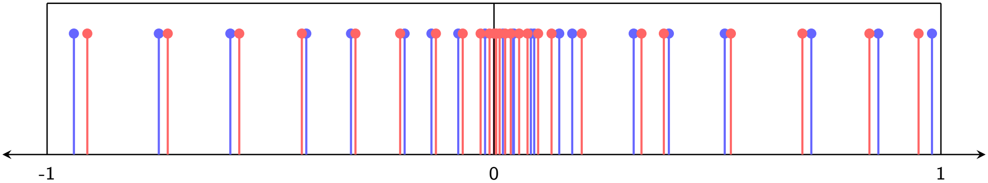
- Lipschitz continuity restriction better understood in the graph and graphon spectral domain

Graphon Spectrum and Convergence of Spectra

- Due to $T_{\mathbf{W}}$ being compact, graphon eigenvalues accumulate at $\lambda = 0$ $\Rightarrow \lim_{i\to\infty} \lambda_i = \lim_{i\to\infty} \lambda_{-i} = 0$

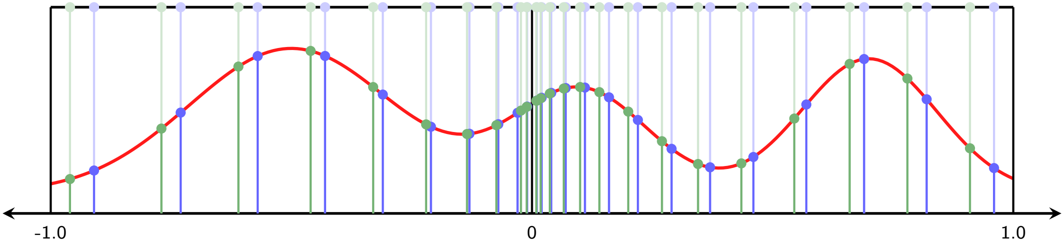
If a graph sequence $\{\mathbf{G}_n\}$ converges to a graphon $\mathbf{W}$, then

$$\lim_{n\to\infty} \frac{\lambda_j(\mathbf{S}_n)}{n} = \lambda_j(T_{\mathbf{W}}) \text{ for all } j$$ (Borgs, C. et al., 2012)



- But for $\neq j$, $\neq n_0$ are needed to show that $\exists\, n_0$ s.t. for all $n > n_0$, $\left|\frac{\lambda_j(\mathbf{S}_n)}{n} - \lambda_j(T_{\mathbf{W}})\right| < \epsilon$

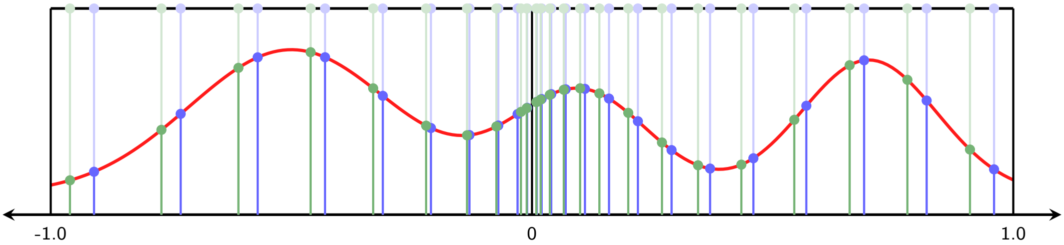
- Because eigenvalues converge, we can expect graph convolutions to converge



- But convergence near $\lambda = 0$ is complicated by eigenvalue convergence not being uniform

- Filters attempting to discriminate spectral components near $\lambda = 0$ do not converge

- This problem can be solved if we amplify these spectral components similarly for $|\lambda| \leq c$



- Lipschitz filters ensure no mismatch between eigenspaces of $|\lambda_j(\mathbf{S}_n)| \leq c$ and $|\lambda_j(\mathbf{W})| \leq c$
- Lipschitz condition means that convergence comes at the cost of spectral discriminability

Lipschitz Graph Convolutions

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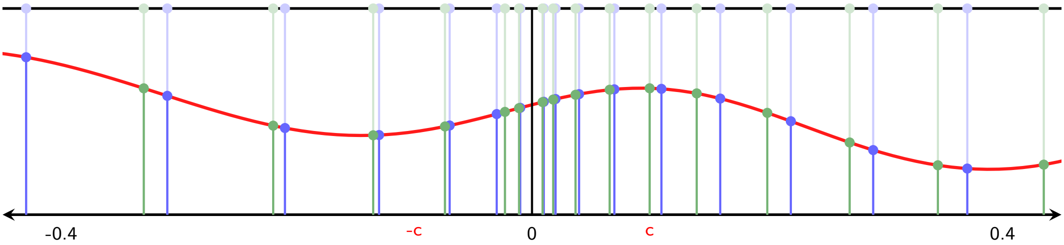

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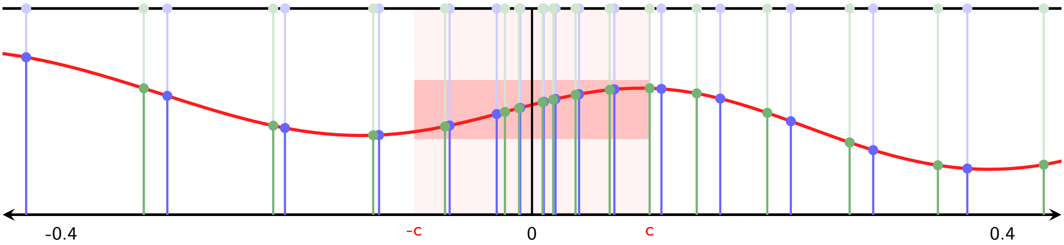

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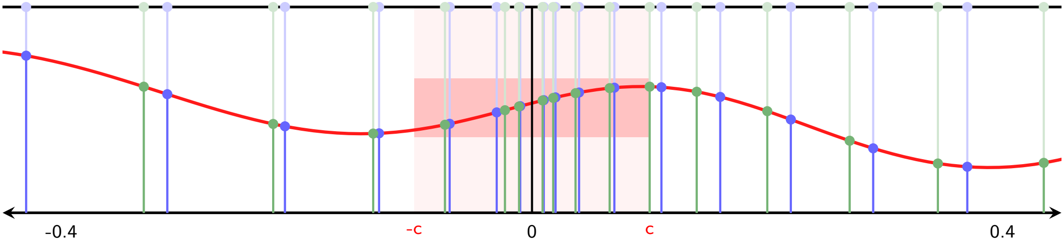
Transferability

- Have established an asymptotic result $\Rightarrow$ graph convolutions converge, but with a condition
- Depending on the value of the Lipschitz constant of $h(\lambda)$, convergence may be faster or slower



- In order to exploit this result in practice, need a non-asymptotic analysis for finite n

Approximating Graphon Convolutions with Graph Convolutions

Theorem (Graphon Filter Approximation) (Ruiz, L. et al., Proc. IEEE'21)

Consider a graph signal $(\mathbf{S}_n, \mathbf{x}_n)$ sampled from the graphon signal (W, X) along with convolution outputs $\mathbf{y}_n = \mathbf{H}(\mathbf{S}_n)\mathbf{x}_n$ and $Y = T_{\mathbf{H}}X$. The difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y\| \leq 2A_w\left(A_h + \pi\frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})}\right)\left(\frac{1}{n}\right)\|X\| + A_x(A_h c + 2)\left(\frac{1}{n}\right) + 2A_h c\|X\|$$

- Bound decreases with n $\Rightarrow$ graph filters better approximate graphon filter for large n as expected
- As $n \to \infty$ we can afford smaller bandwith c $\Rightarrow$ convergence of filters closer to $\lambda = 0$

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- Discriminating around $\lambda = 0$ needs large Lipschitz constant A_h $\Rightarrow$ large approximation error
- Filters that are more discriminative (large A_h) converge more slowly with n $\Rightarrow$ tradeoff

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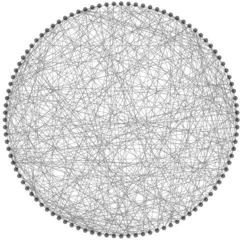
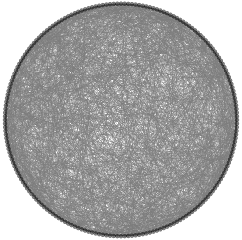
Transferability Paradigm

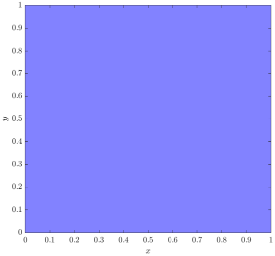
- Consider graphs $\mathbf{G}_n$ and $\mathbf{G}_m$ with $n \neq m$ nodes which are both sampled from the graphon $\mathbf{W}$
- Can upper bound the approximation error between $\mathbf{H}(\mathbf{S}_n)$ and $T_{\mathbf{H}}$. And between $\mathbf{H}(\mathbf{S}_m)$ and $T_{\mathbf{H}}$



n nodes



m nodes



Graphon $W(u, v) = p$

- By the triangle inequality, can upper bound the transferability error between $\mathbf{H}(\mathbf{S}_n)$ and $\mathbf{H}(\mathbf{S}_m)$

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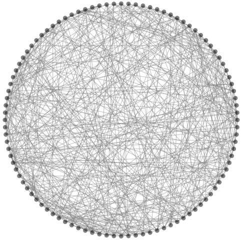

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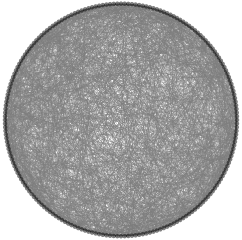

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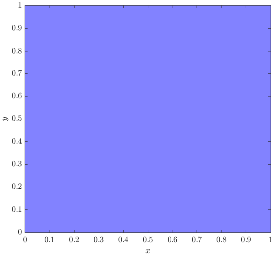

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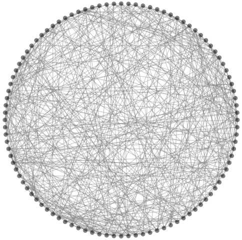

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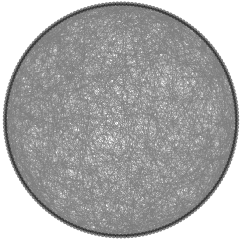

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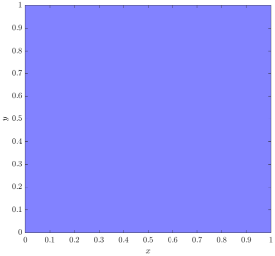

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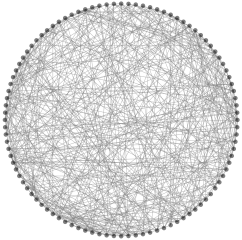

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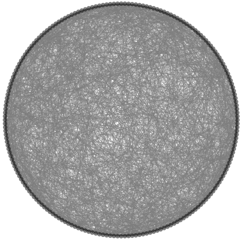
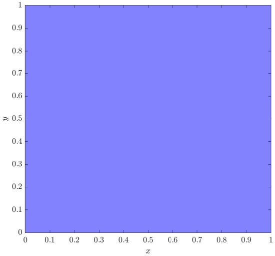


m nodes



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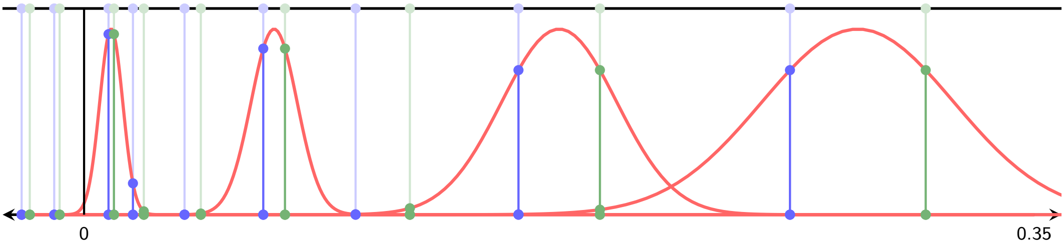
- By the triangle inequality, can upper bound the transferability error between $\mathbf{H}(\mathbf{S}_n)$ and $\mathbf{H}(\mathbf{S}_m)$

Transferability-Discriminability Tradeoff

- If filter is sharp near $\lambda = 0$, spectral components of $\lambda_j(\mathbf{S}_n)$ and $\lambda_j(\mathbf{W})$ are amplified differently



- Transferability and discriminability are not compatible for graph convolutional filters

Graph Neural Networks

Convergence of Graph Convolutions

- So far we have talked at length about graph convolutions and graphon convolutions

$\Rightarrow$ Graph Convolution

$$\mathbf{z}_n = \sum_{k=0}^{K-1} h_k \mathbf{S}_n^k \mathbf{x}_n$$

$\Rightarrow$ Graphon Convolution

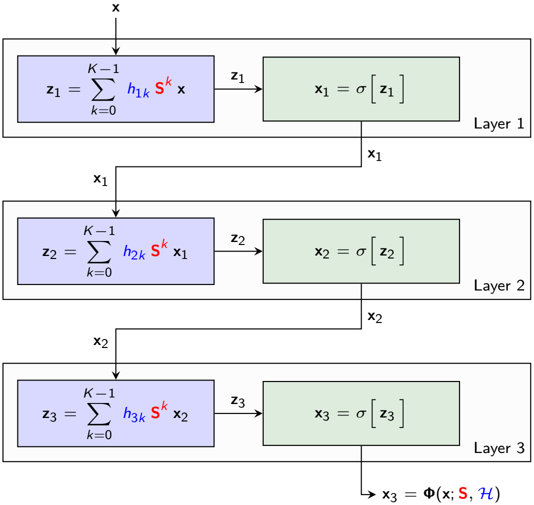
$$Z = \sum_{k=0}^{K-1} h_k T_{\mathbf{W}}^{(k)} X$$

- But we have not talked much about graph neural networks and graphon neural networks

$\Rightarrow$ Graph and graphon NNs are a minor variation of graph convolutions and graphon convolutions

Graph Neural Networks

- A graph NN composes a cascade of layers
- Each of which are themselves compositions
  - $\Rightarrow$ Of graph convolutions $\mathbf{H}(\mathbf{S})$
  - $\Rightarrow$ With pointwise nonlinearities σ
- Define the learnable parameter set $\mathcal{H} = \{h_{kl}\}$
- GNN can be represented as $\mathbf{y} = \mathbf{\Phi}(\mathcal{H}; \mathbf{S}; \mathbf{x})$



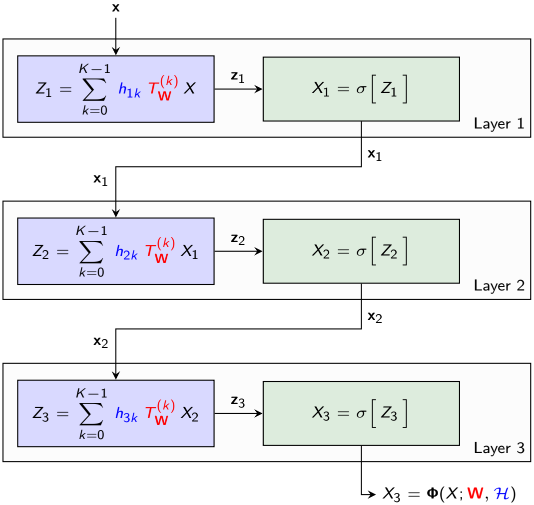
Graphon Neural Networks

- A graphon NN (WNN) composes layers
- Each of which are themselves compositions

  $\Rightarrow$ Of graphon convolutions $T_{\mathbf{H}}$

  $\Rightarrow$ With pointwise nonlinearities σ

- Define the learnable parameter set $\mathcal{H} = \{h_{kl}\}$
- WNN can be represented as $Y = \mathbf{\Phi}(\mathcal{H}; \mathbf{W}; X)$



- The transferability properties of graph filters are inherited by graph neural networks

Theorem (GNN Transferability) **(Ruiz, L. et al., NeurIPS'20, Proc. IEEE'21)**

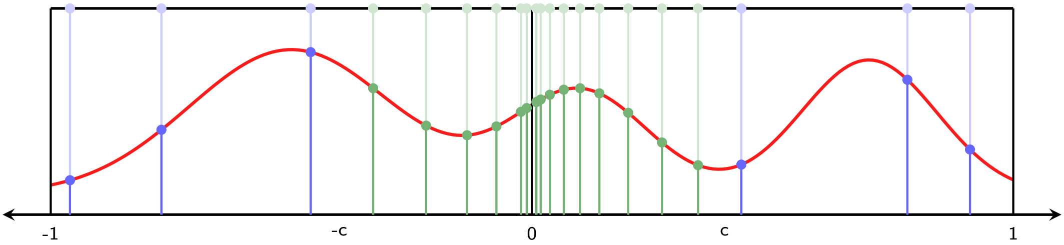
Consider graph signals $(\mathbf{S}_n, \mathbf{x}_n)$ and $(\mathbf{S}_m, \mathbf{x}_m)$ sampled from graphon signal (W, X) along with GNN outputs $\mathbf{y}_n = \Phi(\mathcal{H}; S_n, x_n)$ and $\mathbf{y}_m = \Phi(\mathcal{H}; S_m, x_m)$. The difference norm of the respective graphon induced signals is bounded by

$$\|Y_n - Y_m\| \leq$$

$$LF^{L-1} 2A_w \left(A_h + \pi \frac{\max(B_{nc}, B_{mc})}{\min(\delta_{nc}, \delta_{mc})} \right) \left(\frac{1}{n} + \frac{1}{m} \right) \|X\| + A_x (A_h c + 2) \left(\frac{1}{n} + \frac{1}{m} \right) + 4LF^{L-1} A_h c \|X\|$$

Graph Filters vs. Graph Neural Networks

- The difference in GNNs is that the nonlinearities scatter spectral components all over the spectrum



- Which allows increasing discriminability without hurting transferability. Hence:

$\Rightarrow$ For the same level of transferability $\Rightarrow$ GNNs are more discriminative than graph filters

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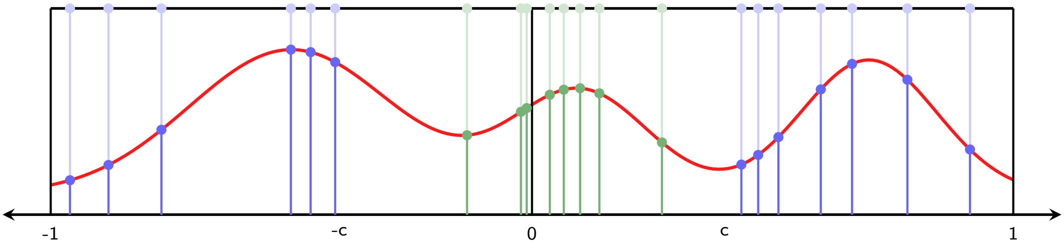

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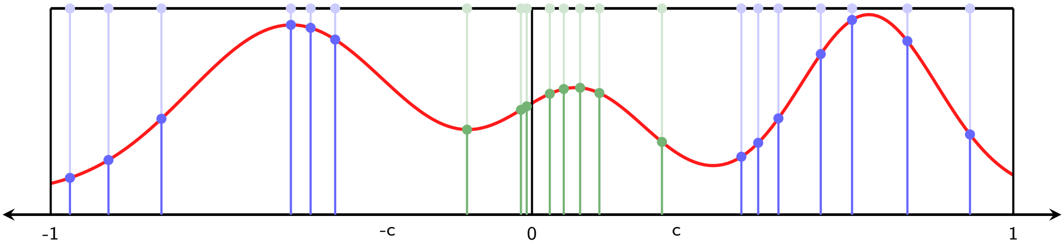

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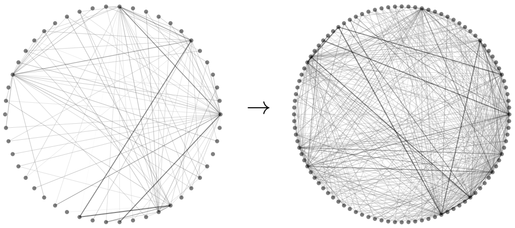
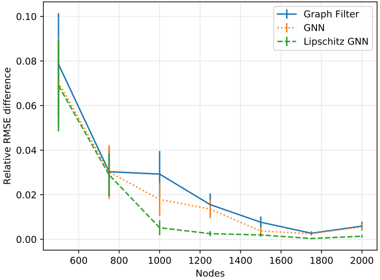
Transferability of Graph Neural Networks

- Transferability of graph neural networks observed empirically $\Rightarrow$ recommendation system

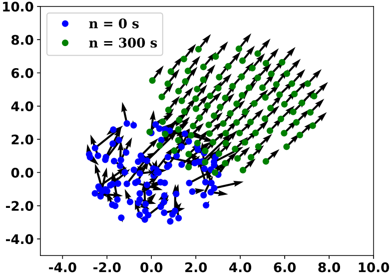


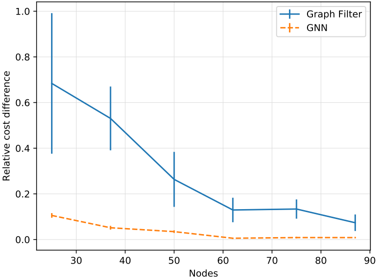


- Performance difference on training and target graphs decreases as size of training graph grows

- GNNs are more transferable than graph convolutional filters. Especially if their filters are Lipschitz

- Transferability of graph neural networks observed empirically $\Rightarrow$ decentralized robot control





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Takeaways

GNNs are more transferable than graph convolutional filters

GNNs are more transferable because of their mixing properties

- Empirical and theoretical evidence support using GNNs for large-scale graph machine learning

Thank you!

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Definitions

- We fix a bandwidth $c > 0$ to separate eigenvalues not close to $\lambda = 0$ and define

(D1) The c-band cardinality of G_n is the number of eigenvalues with absolute value larger than c

$$B_{nc} = \#\left\{ \lambda_{ni} \; : \; |\lambda_{ni}| > c \right\}$$

(D2) The c-eigenvalue margin of of graph G_n is the

$$\delta_{nc} = \min_{i, j \neq i} \left\{ |\lambda_{ni} - \lambda_j| \; : \; |\lambda_{ni}| > c \right\}$$

- Where λ_{ni} are eigenvalues of the shift operator $\mathbf{S}_n$ and λ_j are eigenvalues of graphon W

Assumptions

(A1) The graphon W is A_w-Lipschitz $\Rightarrow$ For all arguments (u_1, v_1) and (u_2, v_2), it holds

$$\left| \mathbf{W}(u_2, v_2) - W(u_1, v_1) \right| \leq A_w \Big(\left| u_2 - u_1 \right| + \left| v_2 - v_1 \right| \Big)$$

(A2) The filter's response is A_h-Lipschitz and normalized $\Rightarrow$ For all λ_1, λ_2 and λ we have

$$\left| h(\lambda_2) - h(\lambda_1) \right| \leq A_h \left| \lambda_2 - \lambda_1 \right| \qquad \text{and} \qquad \left| h(\lambda) \right| \leq 1$$

(A3) The graphon signal X is A_x-Lipschitz $\Rightarrow$ For all u_1 and u_2

$$\left| X(u_2) - X(u_1) \right| \leq A_x \left| u_2 - u_1 \right|$$